

Singularities in kinetic theory

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Abstract: It is revealed that distribution functions of practical gases relate to singularities and such singularities can, with molecular motion, spread to the entire region of interest. It is also shown that even common continuous distribution functions involve a similar quasi-discontinuity difficulty.

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It is widely assumed that the necessary and complete foundation of kinetic theory has been established and the main problem in this field is the lack of powerful computational means: if a sufficiently large supercomputer were available we would be able to solve the well-known Boltzmann-type equations in terms of initial and boundary conditions and the behavior of most practical gases would become analyzable and calculable[1][2]. In view of that similar partial differential equations in fluid mechanics can be handled by today's computers and the obtained results appear to be reasonably good (to a certain extent), it seems that the aforementioned notion concerning kinetic theory is indeed sound and cannot, thus should not, be challenged seriously.

In studying several kinds of gases one, however, found that singularities arose from the standard treatment[3]. Unlike singularities that exist for usual partial differential systems, the observed singularities are not limited to isolated regions; molecular motion carries them to nearby regions as well as distant regions (though collisions between molecules erase them partly). Being exposed to such difficulties, we no longer believe that the principal way of studying kinetic gases is to have Boltzmann-type equations.

The purpose of this paper is to arouse concern for the singularity aspect of the standard kinetic theory. We present realistic examples in that discontinuous distribution functions come to exist and application of differential operator to them becomes risky and misleading. Most of analyses are carried out in terms of solving the collisionless Boltzmann equation numerically and analytically. At the end we briefly discuss in what way we may overcome the difficulties revealed herein.

First of all, let us take a brief look at how the Boltzmann equation can be solved in terms of the standard procedure. The equation reads

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \int [f(\mathbf{v}')f(\mathbf{v}_1') - f(\mathbf{v})f(\mathbf{v}_1)]u\sigma d\Omega d\mathbf{v}_1, \quad (1)$$

where the left side is sometimes called the convective operator and the right side the collisional operator. The detailed meaning of the notations related to two operators can be found in any textbook[1][4]. To solve the differential-integral equation, we must have the initial condition

$$f(t_0 + 0, \mathbf{r}, \mathbf{v}) = f(t_0, \mathbf{r}, \mathbf{v}) \quad (2)$$

and the boundary condition

$$f(t, \mathbf{r}, \mathbf{v}) = \int K(\mathbf{v}, \mathbf{v}_1)f(t, \mathbf{r}, \mathbf{v}_1)d\mathbf{v}_1, \quad (3)$$

where $K(\mathbf{v}, \mathbf{v}_1)$ represents the collisional nucleus between molecules and boundaries[2][5]. According to the existing kinetic theory, these equations, from (1) to (3), constitute a complete equation set to describe the gas dynamics. It is also noted that to numerically solve the equation set a finite-difference scheme based on a grid arrangement in the position-velocity space, such as

$$\frac{\partial f}{\partial t} \sim \frac{\Delta f}{\Delta t}, \quad \frac{\partial f}{\partial x} \sim \frac{\Delta f}{\Delta x}, \quad \frac{\partial f}{\partial v_x} \sim \frac{\Delta f}{\Delta v_x}, \dots, \quad (4)$$

should be employed. If all these are ready, we can, by means of a “true” supercomputer, construct solutions for the equation set. For convenience of later discussion, we will refer to the procedure outlined above, including the equations and all the necessary mathematical treatments, as *the standard solution-construction scheme* of the Boltzmann equation.

Enormous difficulties involve in the solution-construction scheme. What have been well known include: (i) There are seven independent variables: time, geometric coordinates, and velocity components. (ii) The collisional operator is complicated in nature. Due to these difficulties, only much simplified cases have been investigated (one-dimensional cases for instance). In this paper, we put aside these well-known difficulties and try to discuss what may happen when a sufficiently powerful supercomputer is available and a full-dimensional computational job is really performed.

For simplicity, we will disregard collisions between molecules. Nevertheless, the discussion in this paper should hold its significance for rarefied gases as well as for ordinary gases.

Consider a boundary in the gas shown in Fig. 1. Suppose that there initially exists a density difference between the two sides of the boundary and that the density on the left side is much larger. Obviously, molecules on the left side will expand into the space on the right side. At any point on the right side, we will surely find out a certain amount of molecules that come from the left side. By referring to Fig. 2a, we set up a local coordinate system at a point p on the right side in such a way that the y -direction is parallel to the boundary edge and molecules having passed by the edge will move in the x -direction at the point. It is then simple to see that any molecules that have velocities $v_z < 0$ do not come from the left side of the boundary. In Fig. 2b, we schematically plot the velocity distribution at p , which illustrates that the distribution function at $v_z = 0$ involves a discontinuity

$$\frac{\partial f}{\partial v_z} = \infty. \quad (5)$$

If the z -component of the external force is not exactly zero (there is a gravitational force, for instance) the convective operator in the Boltzmann equation fails to make sense at $v_z = 0$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \infty. \quad (6)$$

The situation is rather worrisome since every spatial point on the right side (as well as the left side) of the boundary involves exactly the same singularity for exactly the same reason.

The singularity discussed above has some thing to do with external forces. To have a complete picture, we will, in the remaining part of this paper, investigate examples in that no external force exists.

We consider a gas leaking out of a container through a small hole, as shown in Fig. 3, which schematically represents how a point-size source emits molecules and how the emitted molecules spread out over a free space.

At this point, it is worth mentioning that the situation under consideration is not particularly special. In addition to what happen to leaking gases, there are many practical cases in that molecules behave like an outflow from a point-like source. As shown in Fig. 4, a boundary surface cannot be regarded as a uniform one owing to physical, chemical and geometric differences on it; and this leaves us no choice but to divide the surface into many small, infinitesimally small according to the spirit of calculus, area elements and examine how those elements reflect molecules. Due to the finite temperature of the boundary, the “reflected” molecules from each of the area element will spread as if they are emitted from a small hole. (Emission patterns have been examined by Ref. 5, though from a somewhat different viewpoint.)

We first apply the ordinary fluid mechanics to the fluid around the point p in Fig. 3b. If we further assume that the gas container is rather large, the outflow must be time-independent during the interested period, which means

$$\frac{\partial n}{\partial t} = 0. \quad (7)$$

It is easy to find that at the point p

$$\frac{\partial n}{\partial x} \neq 0, \quad \frac{\partial v_x}{\partial x} = 0. \quad (8)$$

These expressions tell us that the usual fluid equation

$$\frac{\partial n}{\partial t} + \nabla(\mathbf{v}n) = 0 \quad (9)$$

does not hold.

Can the standard kinetic theory do better? The immediate concern is to determine the distribution function related to the gas. By referring to Fig. 3b, in which the origin of the coordinate system is placed at the point-like source, we find that the distribution function can be expressed by

$$f(\mathbf{r}, v, \Omega) = \frac{u(v)g(\Omega)}{r^2} \delta(\Omega - \Omega_{\mathbf{r}}), \quad (10)$$

where Ω is the solid angle of the velocity and $\Omega_{\mathbf{r}}$ is the solid angle of \mathbf{r} in the position space, $u(v)$ stands for a function of $v = |\mathbf{v}|$, which may, for instance, be proportional to $\exp(-\mu v^2/2)$ and $g(\Omega)$ represents a function of Ω . In Eq. (10) the factor r^{-2} is due to the expansion of the molecular paths. It is rather obvious that expression (10) can generally stand for an outflow emitted by a point-size source. In terms of this distribution function, we surely have, at the point p again,

$$\frac{\partial f}{\partial t} = 0, \quad \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0 \quad (11)$$

and

$$\mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} \neq 0. \quad (12)$$

Similar to what happens to the fluid equation (9), the collisionless Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0 \quad (13)$$

is not valid.

When dealing with partial differential equations, it is customary to think of singularity as something isolated in a certain domain. The singularities revealed in this paper, however, are different: the point p in Fig. 3, as well as the point p in Fig. 2, is chosen rather arbitrarily, and this means such singularities exist in the entire space of interest.

To see the deep root of the difficulty, we wish to continue our discussion on one unusual behavior of continuous distribution function. The behavior is well associated with the singularities that have just been discussed.

In Fig. 5, we schematically depict a gas. Suppose that in the shaded region the density of molecules is significantly larger than those in the nearby regions (however, the continuity of the distribution function is still there). Instead of using the standard solution-construction scheme, we try a slightly different, but analytically much more effective, approach. Think about how

the distribution function at the point o influences the distribution function at p_1 and at p_2 . By relating \mathbf{r} and \mathbf{v} in the collisionless Boltzmann equation to those of a moving molecule, we can write the equation as

$$\left. \frac{df}{dt} \right|_{\text{path}} = 0, \quad (14)$$

where the “path” implies that the differentiation is taken along a molecular path in the position-velocity phase space. The solution of Eq. (14) is simply

$$f(t, \mathbf{r}, \mathbf{v})|_{\text{path}} = \text{Constant}. \quad (15)$$

In other words, we can link the distribution function at a certain point to the distribution function at another point if the link exists in terms of a molecule’s path. For the situation shown in Fig. 5a, we know that

$$f(t_0, \mathbf{r}_o, \mathbf{v}) = f(t_1, \mathbf{r}_{p_1}, \mathbf{v}) = f(t_2, \mathbf{r}_{p_2}, \mathbf{v}), \quad (16)$$

where \mathbf{v} is the velocity of the moving molecule (no external force exists). In terms of (16), we may say that o is the “source” point and p_1 or p_2 is the “image” point.

The formulation above seems “exactly” consistent with the standard approach. However, there are several things worth special mentioning. As one thing, the path-information of molecules plays an active and essential role in this approach while it is considered almost irrelevant in the equation set (1)-(3). As another thing, this approach is less sensitive to singularities. Equation (14) is an ordinary differential equation along a path and the singularities associated with (5) and (6), for instance, do not spell much trouble to it.

The resultant expression (14) or (15) brings out that, by referring to the Fig. 5b, the local distribution functions at p_1 and p_2 have cone-like structures. The structures are interesting in the following two senses. One is that the cones become sharper and sharper constantly as the distance between the source and the image increases. The other is that though the initial variation of the distribution function is in the spatial space, the cone-like structures are formed later on in the velocity spaces of other points.

In Fig. 6, we plot the distribution function versus the polar angle in the velocity space. The figure clearly illustrates that with the increase of the distance between the source and the image

$$\frac{\partial f}{\partial \theta} \rightarrow \text{very large}. \quad (17)$$

If the expression

$$\frac{\partial f}{\partial \theta} \rightarrow \infty \quad (18)$$

is allowed to characterize a true discontinuous distribution function, see for instance expression (10), it should be appropriate to name the feature related to (17) as the *quasi-discontinuity*.

It is now in order to comment on the applicability of the standard solution-construction scheme outlined at the beginning of the discussion. Equation (17) has shown that even if we assume that the distribution function under consideration is initially continuous and the gas is free from boundary effects, the standard scheme will still encounter difficulties. As the cones of the velocity spaces become sharper and sharper, too sharp to be described by the chosen grid arrangement, some kinds of δ -functions have to be employed. In this sense, no approach is truly usable unless a way is included in which both continuous and discontinuous distribution functions are treated on a roughly equal footing.

Finally, we make a brief examination of possible direction in which the revealed difficulties can be surmounted.

The discussions in this paper have shown that the most essential task is to deal with continuous and discontinuous distribution functions in a unifying way. After many unsuccessful tries, we are convinced that the task can be accomplished by an integral procedure in that the path-information of molecules plays an important role. The reasons for that include: (i) Integral operations, unlike differential operations, are usually not sensitive to discontinuity; if formulated adequately, the behavior of both discontinuous and continuous distribution functions can be described. (ii) In discussing the discontinuity and the quasi-discontinuity, we have seen that if the path-information of molecules is made of use, the mental picture, as well as the resultant formulas, becomes much clarified.

Based on the conceptions aforementioned, we have developed a path-integral approach[3][6] in that the singularity difficulties revealed in this paper are removed. Best of all, some of full-dimensional practical gases become calculable in terms of today's computers.

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Figure captions

1. A gas in that density difference is maintained by boundary blocking.
2. Discontinuous distribution function associated with boundary blocking. (a) The local coordinate frame at a point p . (b) The distribution function versus v_z .
3. A gas leaking out of a container through a small hole.
4. Schematic of molecules reflected by a boundary.
5. A dense gas influencing the nearby and distant regions.
6. Distribution function in terms of the polar angle. (a) In a nearby region. (b) In a distant region.

Figure 1

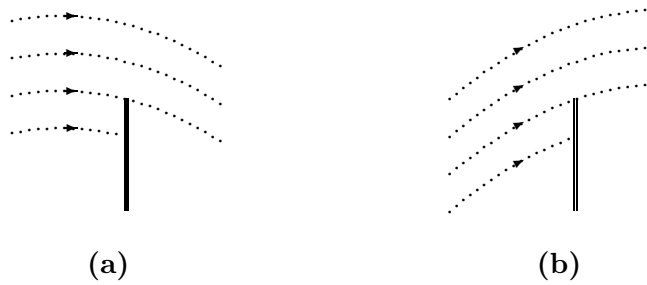


Figure 2

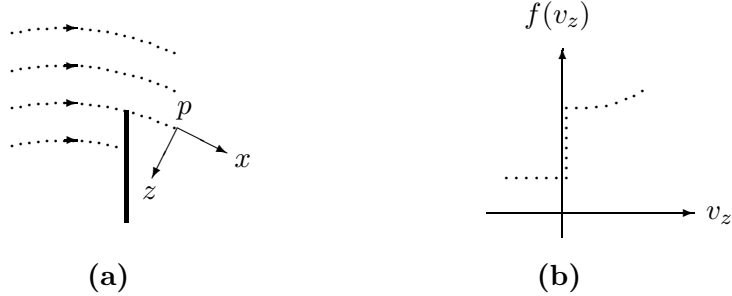


Figure 3

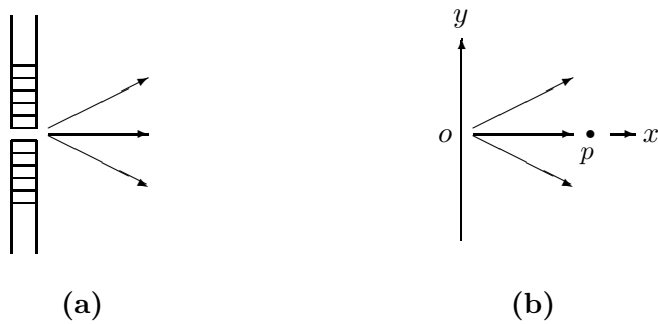


Figure 4

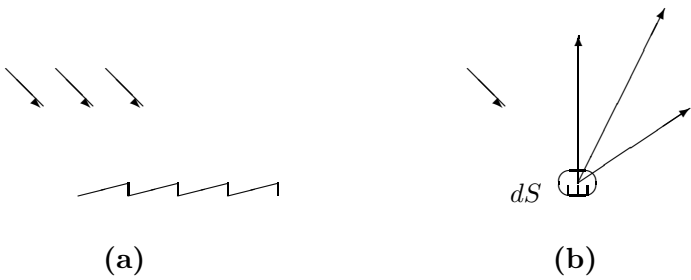


Figure 5

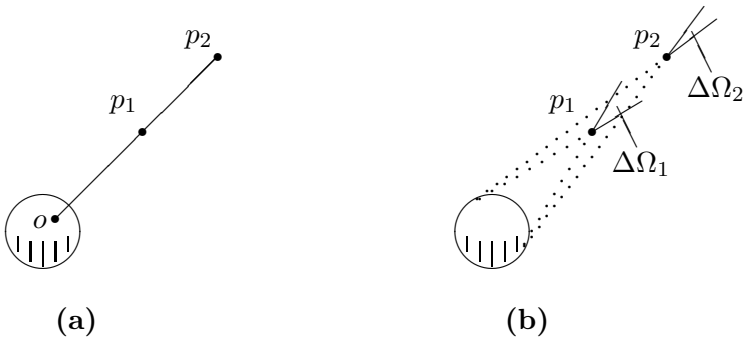


Figure 6

